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13. SUPPLEMENTARY NOTES

14. ABSTRACT

A computer system comprising 32 nodes and 64 processors was purchased and installed along with necessary peripherals and software. This system is currently supporting research being done under grant #F49620-03-1-0046.

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Final Report
August 31, 2003
Conformations of Macro Molecules
AFOSR Grant F49620-02-1-0215
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I. Introduction

This grant was awarded under the Defense University Research Instrumentation Program (DURIP) in support of ongoing research funded by AFOSR and other agencies. These include AFOSR grants F49620-9-1-0048, which was in force at the time the DURIP was funded, the subsequent renewal of that grant F49620-03-1-0046, and a number of grants sponsored by NSF. Our research program, as detailed in the various proposals and annual reports, involves both experiment and extensive theoretical modeling. At the time the DURIP proposal was written the modeling for a specific system would often lag weeks to months behind experiment due to our limited computing resources. A case was made in the proposal for substantially increasing those computing resources in order to bring experiment and theory/modeling into the same time frame. This would allow them to effectively interact and the research could be more efficiently and expertly completed. The proposal was funded and the system briefly described below was purchased.

II. Progress

It was decided not to continue the workstation model that we had used up to the funding of this grant. Due to tremendous improvement in the speed and capacity of PC-modules we decided to build a multinode system where each node contained two independently addressable ultrafast processors. At the time we wrote the proposal we designed a system composed of a master node and 22 dual processor nodes. Each processor would operate at 1.2 GHz, have 512 MB RAM and a 9.1 GB hard drive. In addition, we requested funds for two graphics work stations and some updated software.

Once the proposal was funded we decided to proceed in two steps. This was done for a number of reasons. First, it was clear that in the year that elapsed from submitting the proposal to receiving the funds great strides had been made in processor speed and hard drive capacity. Second, we had no experience with multinode systems so we decided to only build half the system first but do it anticipating expansion in the future. Due to price reductions and processor improvement we started with a 16 node, 32 processor unit where each processor operated at 1.9 GHz and had a 40 GB hard drive. This system has a computing capability in excess of the entire system envisioned when the proposal was written. A further 1.9 GHz dual processor was designed as a server node with 1.0 GB RAM and dual 35 GB SCSI hard drives. This server had sufficient capacity to allow future expansion.

Components were received and assembled approximately 3 months after the grant became active. It took another month or so to install all of our software and to write the scripts necessary for job submission; queuing, etc. The result was spectacular.

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Within about 6 weeks we had eliminated a 3 month backlog of jobs and could begin analyzing and modeling data in "real time". The presence of this machine also allowed us to begin to envision modeling as a way to lead and evaluate potential experiments before they were run to see if potentially useful results could be obtained. While still remaining strongly rooted in experiment, PRION (our name for this system) allowed rational experimental design and more fruitful interactions with our synthetic colleagues.

We evaluated PRION for about 6 months before deciding what to do with the remainder of the DURIP funds. In the end we decided doubling the existing system was the best way to go. We had made substantial investment in "learning" how to use PRION effectively, including writing numerous scripts for specific problems, and in 6 short months had succeeded in saturating the system. Hence, we purchased another 16 dual processor nodes only this time they ran at 2.4 GHz, a 25% increase in speed. We also bought the graphics work stations, ending up with four instead of the original two. A backup node was purchased that continually backed up the 32 nodes now comprising PRION. The full system came on line in August, 2003 and is working beautifully.

In all, PRION is very good value for money, supporting several million dollars worth of experiment and a significant research team for under $80,000. It is more than meeting our current needs. However, we can already see as we move into larger systems the need for a companion to PRION that will operate in parallel with ultrafast internal communication between processors. That is for a future DURIP proposal, however, when once again the need to upgrade our computing resources will be urgently needed.